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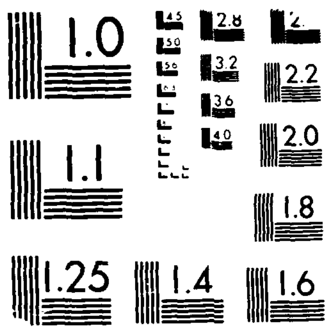

MICROCOPY RESOLUTION TEST CHART

IREAU STANDARDS 1963 A

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We show that the acoustic branches calculated by our helical lattice dynamics calculations can match the observed inelastic neutron scattering results. The fit in the neutron sub Terrahertz region is consistant with our fit to Brillouin results in the Gegahertz region when the frequency dependence of the dielectric constant of water is taken into account.

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Revised version

Helical Lattice Vibrational Modes in DNA

A recent letter by Grimm et al.[1] reported the observation of umklapp-phonon scattering at sub teraHertz frequencies in DNA by inelastic neutron scattering. They found, that the nearly linear dispersion of their results did not extrapolate to zero frequency at zero wavevector as a simple acoustic mode should and that the data could be best fit by a dispersion relation $\omega^2 = \omega_o^2 + v^2(\Delta Q)^2$ where $\omega_o/2\pi$ was 0.4 THz. This is in disagreement with two earlier observations[2,3] carried out by Brillouin scattering, between 5-20 GHz, where the acoustic mode is seen to behave normally and extrapolate to zero frequency at zone center. We point out, that a proper helical lattice dynamics analysis of vibrational modes of the DNA helix resolves this apparent inconsistency, and that the inelastic neutron data as well as the Brillouin data are in excellent quantitative agreement with such calculations.

The lowest optical mode at zone center in Fig. 1 has been observed experimentally[4], as well as other optical modes calculated by the lattice theory.[5] As seen in Fig. 1 the lowest longitudinal acoustic branch does extrapolate linearly to zero frequency at zone center. The Brillouin observations in the GHz region fall on this branch. The heavy lines indicate the continuation of the compressional character of the phonons on the successive branches of the dispersion plot of Fig. 1. The experimental resolution is such that the splitting of the branches near the crossover cannot be seen. We note that a feature exists in the experimental data near the second from bottom optic-acoustic crossover that is consistent with the predicted region of crossover.

The value of the acoustic velocity from this calculation is 4.5 km/s. To compare with the Brillouin work in the GHz region, we changed the long range water dielectric to 45 (from 9) and calculated an acoustic velocity of

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3.1 km/s. This is about what would be expected for a helix unburdened by water of hydration, based on measurements by Lee et al.[6]

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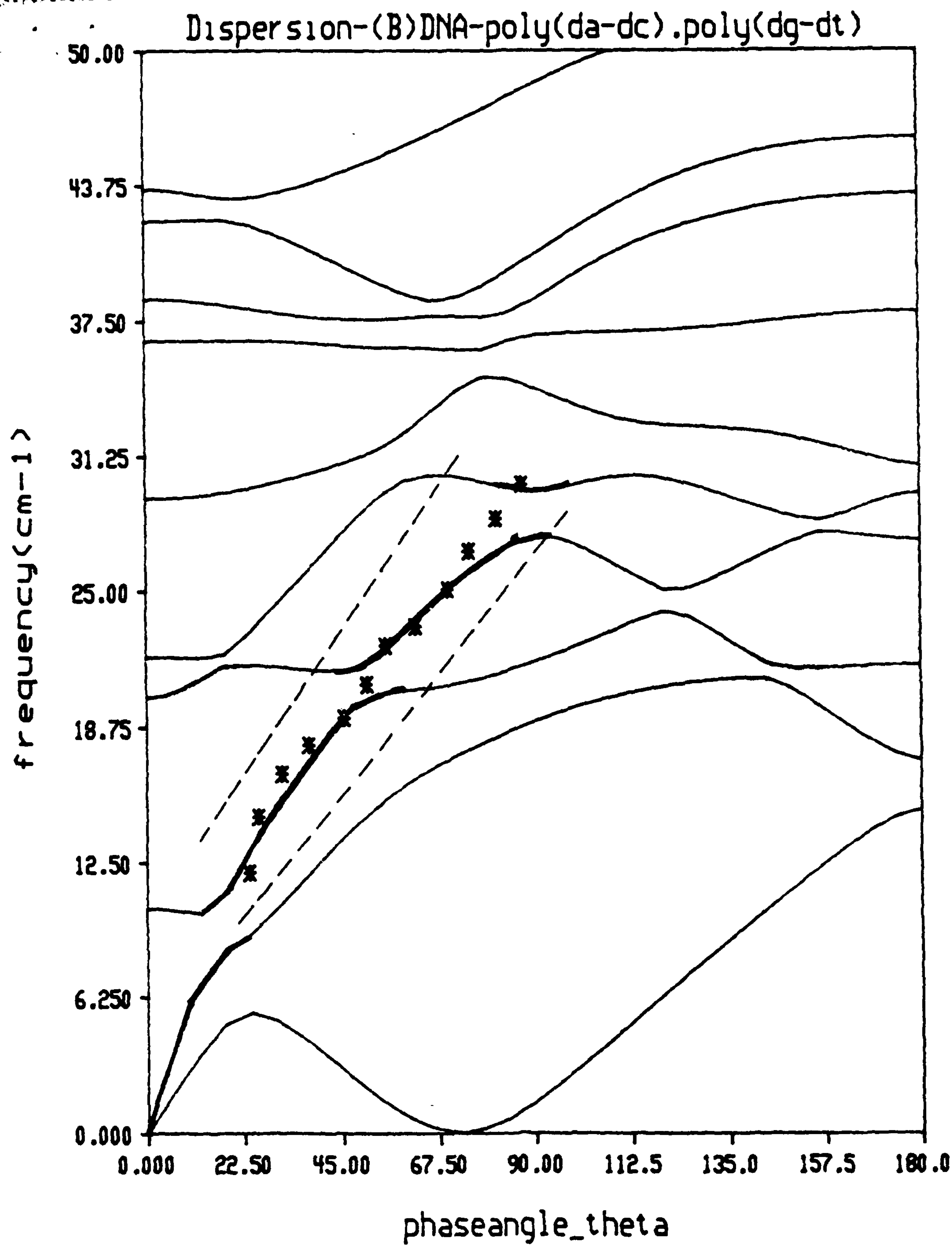
Figure Captions

Fig. 1 The continuous lines are our helical lattice dispersion calculations of the phonon spectrum of DNA. The θ axis is displayed in degrees of phase shift from one unit cell of two DNA base pairs to the next. The central row of stars show the reported frequencies from the neutron data and the outer rows of dashes show the reported FWHM line width. The heavy lines indicate the continuation of the compressional character of the phonons on the successive branches of the dispersion plot.



Dispersion-(B)DNA-poly(da-dc).poly(dg-dt)
frequency(cm-1)
50.00
43.75
37.50
31.25
25.00
18.75
12.50
6.250
0.000
0.000
22.50
45.00
67.50
90.00
112.5
135.0
157.5
180.0
phaseangle_theta

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